

Trimethyl phosphate

512-56-1 | DTXSID1021403

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.64 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.42e-01

Confidence level: 7.24e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Trimethyl phosphate</div> <div>Measured: 3.57</div> <div>Predicted: 3.64</div>	<div>Image not found</div> <div>Ethyl dimethyl phosphate</div> <div>Measured: 3.24</div> <div>Predicted: 3.42</div>	<div>Image not found</div> <div>Dimethyl propyl phosphate</div> <div>Measured: 2.97</div> <div>Predicted: 2.43</div>
<div>Image not found</div> <div>Dimethyl methylphosphonate</div> <div>Measured: 8.06</div> <div>Predicted: 6.36</div>	<div>Image not found</div> <div>Triethyl phosphate</div> <div>Measured: 2.74</div> <div>Predicted: 1.41</div>	